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Title: Deep ML for inference from indirect measurements

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Deep ML for inference from indirect measurements

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The magic of deep machine learning (DML)

- Neural networks that can beat Go grandmasters
- Networks that have better than human accuracy at classifying images in over 100 categories
- Making still pictures move realistically
- Super-resolution versions of very old film clips
- Realistic, high-resolution, images of people that have never existed
- Realistic insertion of people into video clips
- Network generated music and writing that passes for human created
- How can this technology be leveraged for physics and engineering?

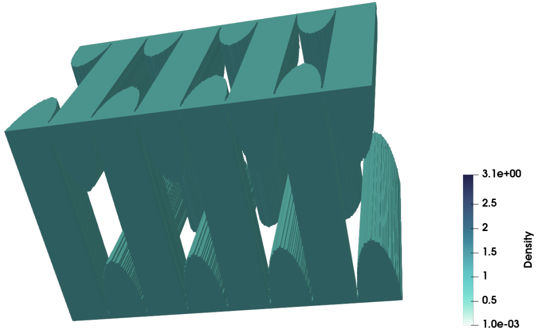
Not a real person. At least, as far as we know.

Outline

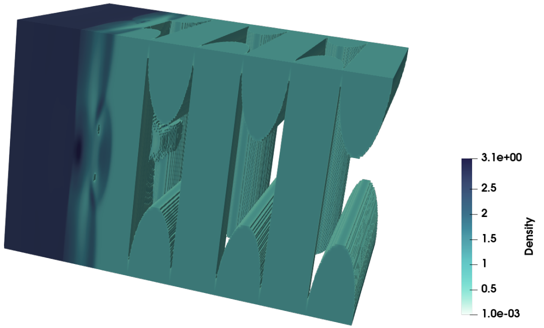
1. Introduction of an example problem for deep ML
2. Background on methods for inverse problems
3. Overview of ”data-driven” methods
4. How deep ML changes the landscape
5. Inference of relative strength from shock radiographs
6. Analysis of deep ML inference
7. Open questions

Shocks in additively manufactured materials

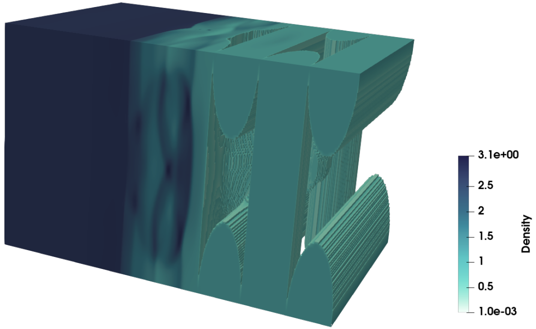
- Additively manufactured structures are being investigated for use in production roles
- Printed materials can have highly varying material properties
- Complex structures can yield interesting response properties
- We investigate one type of these materials undergoing high-velocity impact



T_0



T_1

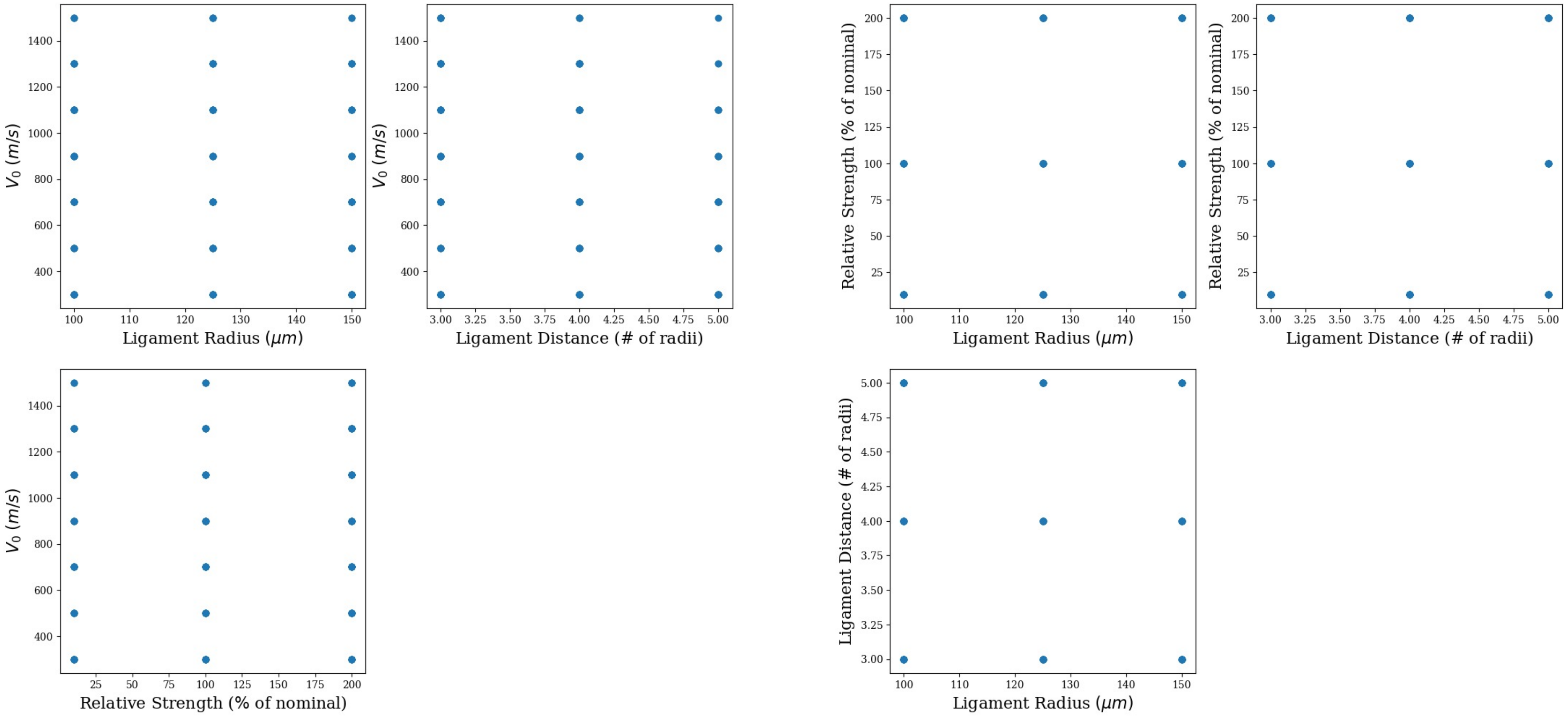


T_2

Shocks in additively manufactured materials

- Data set consists of 155 Ale3D simulations
- Shock through 3D structure over $1\ \mu s$ sampled every $0.025\ \mu s$
- Parallel-beam radiograph generated at every timestep
- Simulations varied:
  - Ligament radius
  - Ligament spacing
  - Impact velocity
  - Relative strength of ligament material
- Result is 6355 radiograph images
- **We focus on inferring the ligament strength from the radiograph**

Shocks in additively manufactured materials



Methods for inverse problems

- Inverse problems focus on calculating causal factors from observations
- Inverse problems are often ill-posed
- Hadamard's well-posedness
  1. A solution exists
  2. The solution is unique
  3. The solution depends continuously on the data
- Example: Radon transform in X-ray imaging
- Forward model of X-ray data is well-posed
- Despite a direct inverse formula, experimental sampling can make reconstructing the absorption ill-posed

$$Rf(t,\omega) = \int_{\mathbb{R}} f(t\omega + s\omega^{\perp})\, ds$$

The Radon transform

$$f(x) = \frac{1}{4\pi^2} \int_0^{\pi} \int_{\mathbb{R}} e^{ir\langle x,\omega\rangle} \widetilde{Rf}(r,\omega) |r|\, dr\, d\omega$$

Direct inversion of Radon transform

Methods for inverse problems

- To deal with ill-posedness and noise in measurement a variational approach is often used
- The forward map, $\mathcal{T} : X \to Y$, yields the data $g = \mathcal{T}(f_{\mathrm{true}}) + \delta g$
- A loss function, $\mathcal{L} : Y \times Y \to \mathbb{R}$, characterizes the agreement of a reconstruction, f, with the data, g
- Example: $\mathcal{L}(\mathcal{T}(f), g) = \|\mathcal{T}(f) - g\|_2^2$
- Regularizer, $\mathcal{S} : X \to \mathbb{R}$, adds *a priori* constraints on reconstruction
- Example: $\mathcal{S}(f) = \|f\|_{TV} = \||\nabla f|\|_1$

- Variational methods then solve the optimization

$$\min_{f \in X} \left[\mathcal{L}(\mathcal{T}(f), g) + \lambda \mathcal{S}(f)\right] \text{ for a fixed } \lambda \geq 0$$

Methods for inverse problems

- Variational methods:
  - Make the problem less ill-posed
  - Add prior information not in data
- Variational methods do not:
  - Characterize non-uniqueness
  - Characterize effect of observation noise
- Instead formulate the variational optimization as a Bayesian posterior distribution
  - Likelihood:

$$p(g|f) = \exp\left(-\mathcal{L}(\mathcal{T}(f), g)\right)$$

  - Prior:

$$p(f) = \exp\left(-\lambda \mathcal{S}(f)\right)$$

  - Posterior:

$$p(f|g) \propto p(g|f)p(f)$$

The "data-driven" approach to inverse problems

- With deep ML we can process 10^6 high-dimensional data points to learn mappings
- With access to the forward map, $\mathcal{T} : X \to Y$, we can generate large samples of (f, g) pairs. Training datasets.
- A neural network can then learn the mapping:

$$\mathcal{T}^{-1} : g \mapsto f$$

- *A priori* information is encoded by sampling, $f \in \mathcal{M}$
- Learn the restricted mapping:

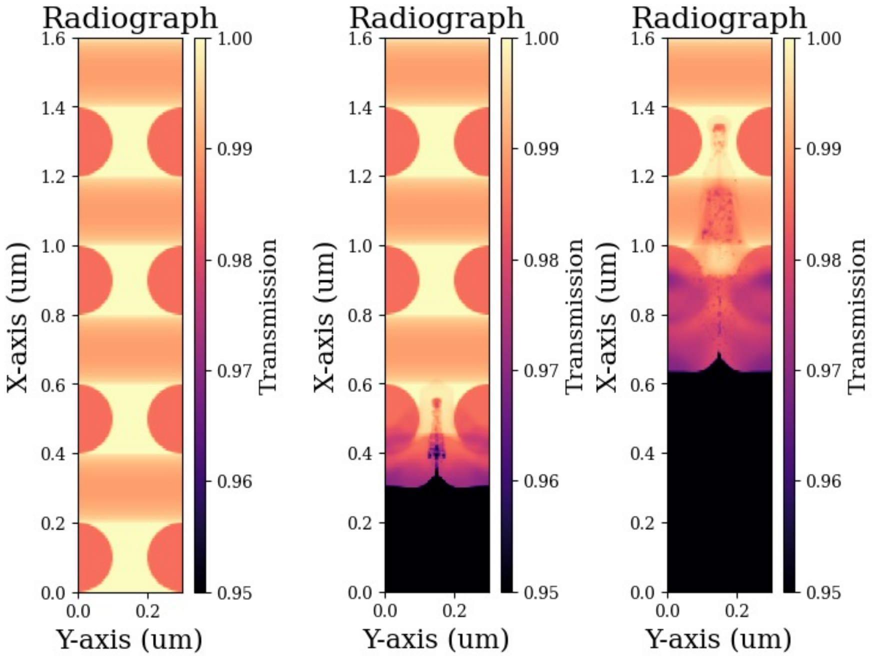
$$\mathcal{T}_{\mathcal{M}}^{-1} : g \mapsto f \in \mathcal{M}$$

The “data-driven” approach to inverse problems

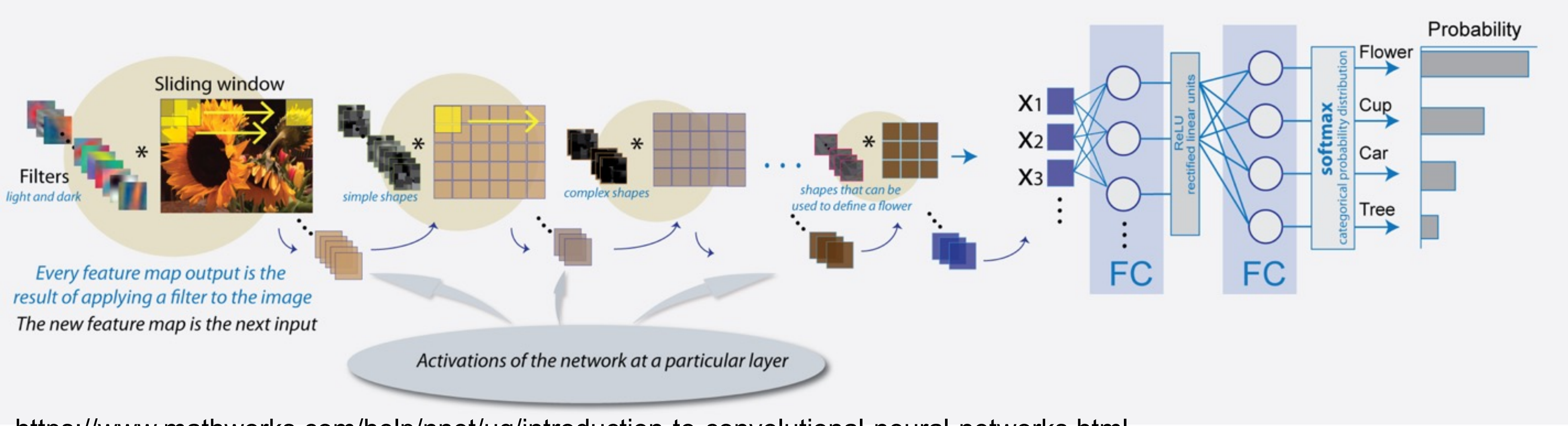
- Advantages over variational and Bayesian approaches
  - Can encode much more complex a priori information through sampling
  - Optimization does not have to be performed for each new data point
  - Regularization parameters do not have to be tuned
  - Can solve the problem for multiple a priori conditions simultaneously
- Difference between physical inverse problems and standard DML application domains
  - In imaging challenges, extrapolation outside of the sample manifold is not expected
  - Many DML results are subjective (e.g. ”Does this image or video look real?”)
  - When generating training data from physics simulation there is often model error from experimental observation
  - For physical experiment, observation data can be extremely limited.

Inferring relative strength from radiographs

- We try to learn relative strength from a radiograph
- Input:
  - Radiograph (256 x 512)
  - XY-pixel size
  - Observation time
  - Ligament radius
  - Ligament spacing
  - Impact velocity
- Output:
  - Relative Strength
- Training considerations:
  - Training, Validation, Testing (TVT) split: 70/20/1
  - Batchsize: 8 data points used for each gradient descent step
  - Learning rate: Optimization step scaled by 0.001



What is a convolutional layer?



https://www.mathworks.com/help/nnet/ug/introduction-to-convolutional-neural-networks.html

- Filters are not prescribed, instead ”learned” by fitting to training data
- Separate image “channels” are convolved and output is added for each convolutional layer output
- Addition of non-linear activation makes them much more than a traditional convolutional filter

Inferring relative strength from radiographs

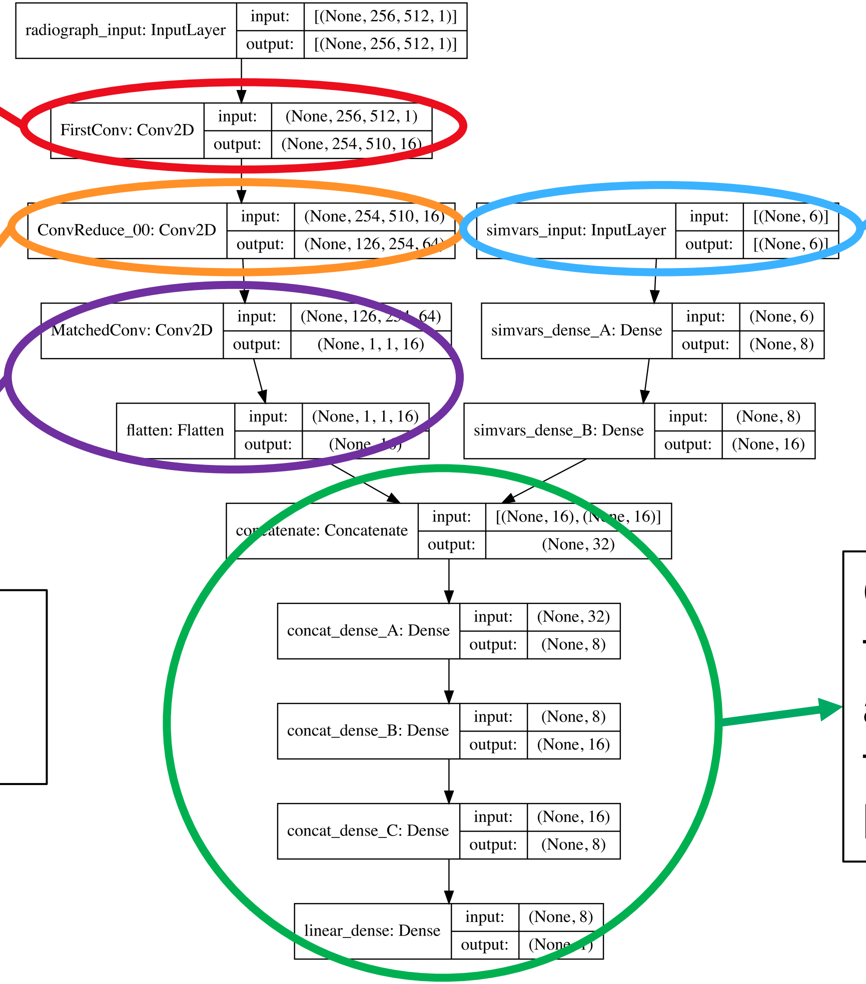
Radiographs fed to initial convolution

Repeated convolutions that halve image size

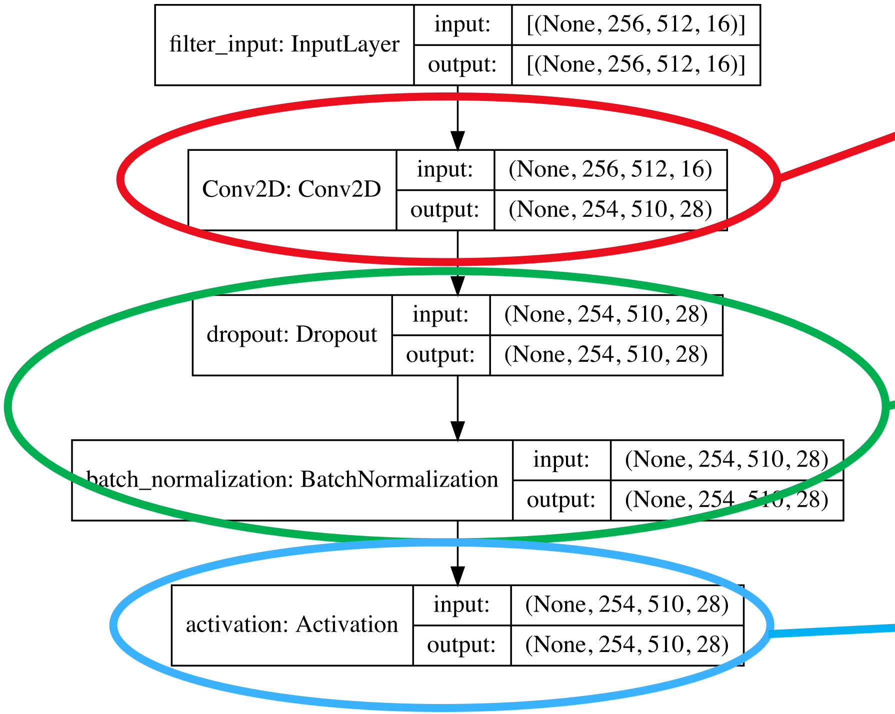
Matched filter to convert image to vector

Input of conditional variables followed by dense layers

Concatenation of filtered radiographed and processed inputs followed by dense layers



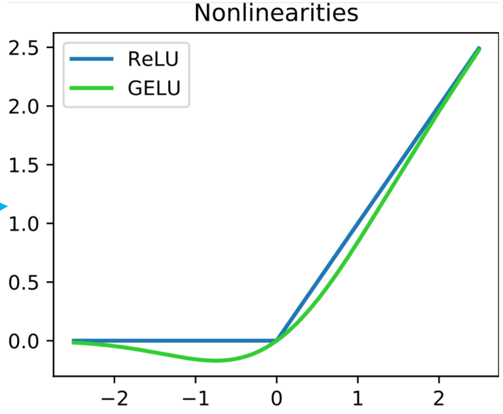
Inferring relative strength from radiographs



Standard 2D convolution

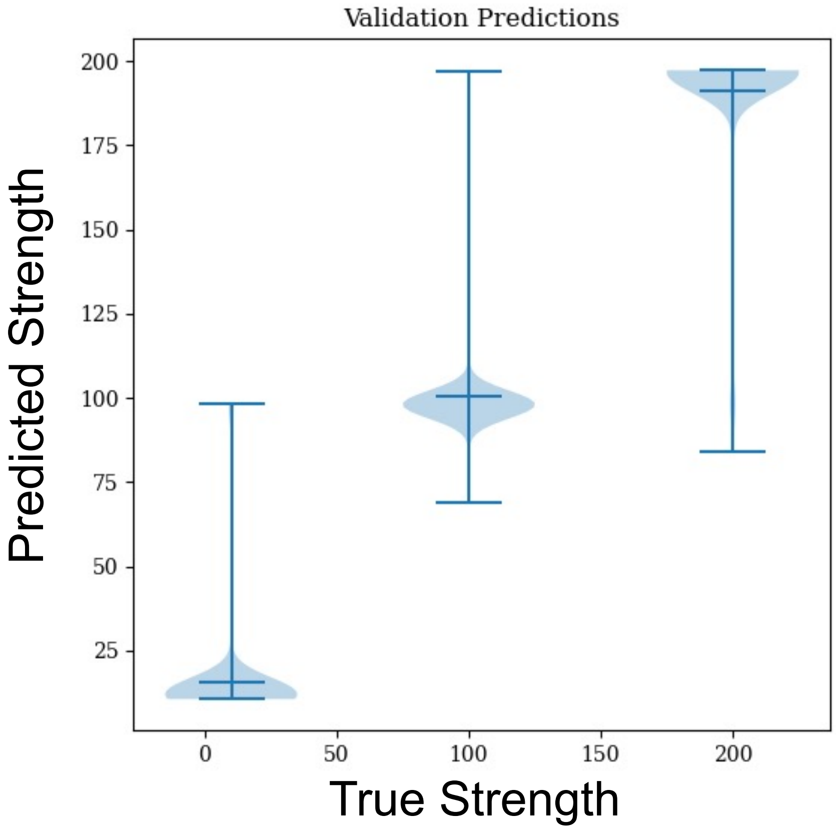
Regularization using dropouts and batch-normalization

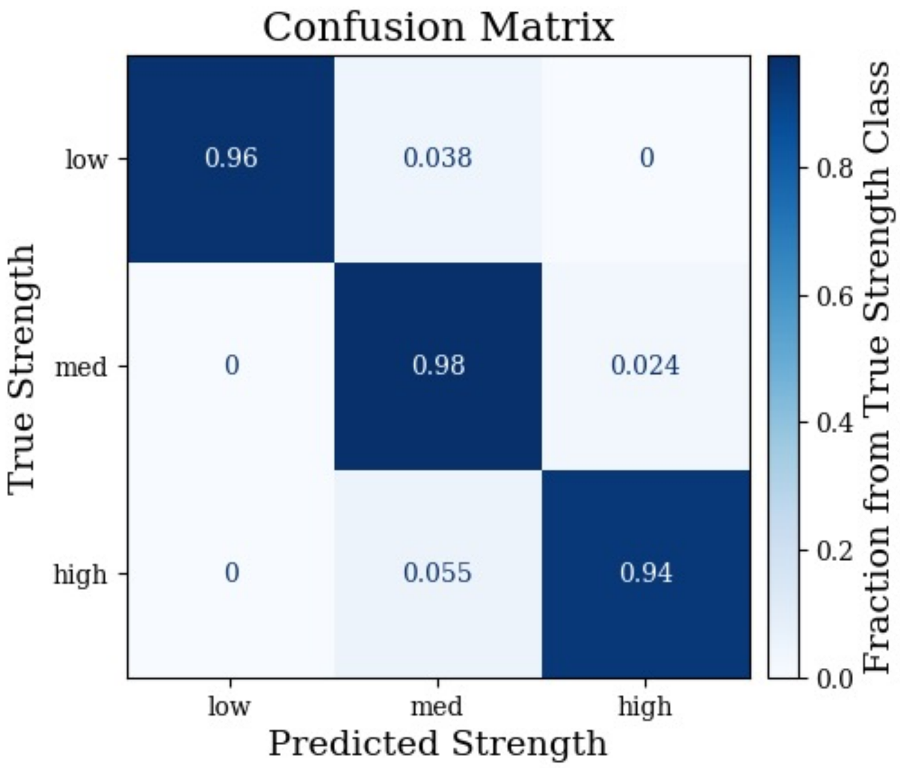
Components of a standard "convolutional layer"



upload.wikimedia.org/wikipedia/commons/4/42/ReLU_and_GELU.svg

Inferring relative strength from radiographs





Open questions for deep ML applications to physics inference

- When the experimental data is sparse, how do you characterize simulation error?
- If simulations form our training sets can we use deep ML to discover new physics models?
- How stable are the features learned through the neural network approach?
- How do we know if an inference problem is tractable without training a network?
- How do quantify the “optimality” of a network architecture?